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Studies on Electronic Structure and Magnetic Properties of an Organic Magnet with Metallic Mn^{2+} and Cu^{2+} Ions

YAO Jian-Guo[1] and PENG Guang-Xiong[2]

[1] Department of Basic Sciences, Hubei Automotive Industries Institute, Shiyan 442002, China
[2] Institute of High Energy Physics, the Chinese Academy of Sciences, Beijing 100039, China
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Abstract: The electronic structure and the magnetic properties of the non-pure organic ferromagnetic compound $MnCu(pbaOH)(H_2O)_3$ with pbaOH = 2-hydroxy-1, 3-propylenebis (oxamato) are studied by using the density-functional theory with local-spin-density approximation. The density of states, total energy, and the spin magnetic moment are calculated. The calculations reveal that the compound $MnCu(pbaOH)(H_2O)_3$ has a stable metal-ferromagnetic ground state, and the spin magnetic moment per molecule is 2.208 μ_B, and the spin magnetic moment is mainly from Mn ion and Cu ion. An antiferromagnetic order is expected and the antiferromagnetic exchange interaction of d-electrons of Cu and Mn passes through the antiferromagnetic interaction between the adjacent C, O, and N atoms along the path linking the atoms Cu and Mn.

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Key words: density-functional theory, non purely organic magnet, electronic structure, ferromagnetic properties

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